Three-dimensional multiwell phase-field model for athermal ω in Ti–Mo with a realistic chemical background

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Athermal β → ω transformation in Ti–Mo alloys produces a multivariant microstructure with four ω variants. We build on our recent multiwell phase-field model for total spreading [1], in which a double-ditch term in the interfacial energy suppresses direct contact between different ω variants, keeping them separated by thin layers of the parent β phase. The four ω variants are described by order parameters, while the β phase follows from the sum-to-unity constraint. Here, we extend this framework by including fully anisotropic elasticity with phase-dependent stiffness tensors, a chemical driving force computed from the local molybdenum concentration and temperature through the Gibbs free energies of the β and ω phases [2], and a Langevin noise term representing thermal fluctuations and enabling nucleation from an initially β state. The molybdenum field is obtained by atomistic preprocessing with realistic short-range order and projected onto the computational grid.

We apply the model to cooling of a Ti–15Mo sample studied by in-situ synchrotron X-ray diffraction. The experiment resolves the parent β phase, four ω variants associated with the four $\langle 111 \rangle_\beta$ directions, and a transition phase related to incomplete β → ω shuffle. Three-dimensional large-scale simulations in a periodic cube of side 42 nm with a realistic molybdenum background reproduce preferential nucleation of ω in chemically favorable regions, subsequent growth of the four variants, and their separation by the β phase, see Figure 1. The simulations show good agreement with the experimentally observed evolution during cooling.

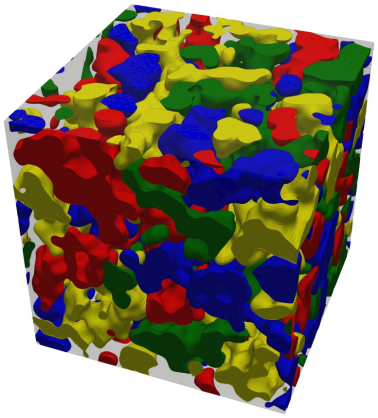

Figure 1: Snapshot of the simulated β → ω transformation in Ti–15Mo during cooling at 200 K. The four colors denote the ω variants, which remain separated by the parent β phase (transparent).

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[1] J. Kozlík, K. Tůma, O. Souček, J. Dobrzański, S. Stupkiewicz, *Multiwell phase-field model for arbitrarily strong total-spreading case*, International Journal of Engineering Science **221**, 104474, 2026.

[2] J.Y. Yan, G.B. Olson, *Computational thermodynamics and kinetics of displacive transformations in titanium-based alloys*, Journal of Alloys and Compounds **673**, 441–455, 2016.